



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 8SG3 / pdb_00008sg3
Title : High Affinity nanobodies against GFP
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Deposited on : 2023-04-11
Resolution : 3.11 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

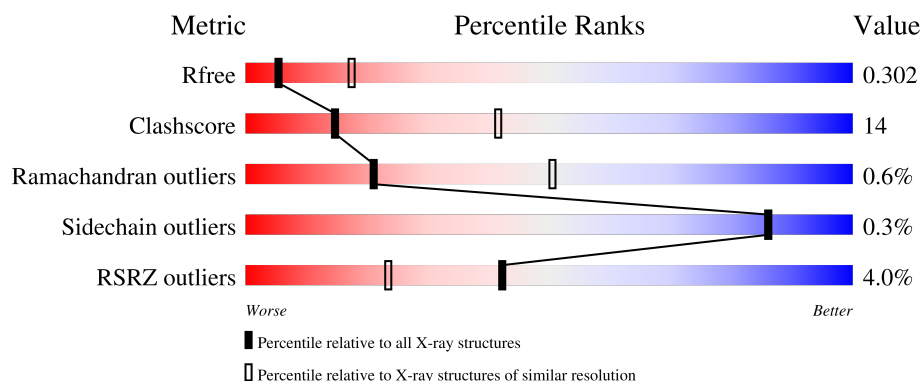
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	253	3% 66% 23% 10%
2	B	141	4% 64% 23% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5445 atoms, of which 2666 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	227	Total	C	H	N	O	S	0	0	0
			3556	1157	1740	307	346	6			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	insertion	UNP P42212
A	66	CR2	SER	chromophore	UNP P42212
A	66	CR2	TYR	chromophore	UNP P42212
A	66	CR2	GLY	chromophore	UNP P42212
A	72	ALA	SER	conflict	UNP P42212
A	177	HIS	GLN	conflict	UNP P42212
A	239	GLY	-	expression tag	UNP P42212
A	240	LEU	-	expression tag	UNP P42212
A	241	GLU	-	expression tag	UNP P42212
A	242	VAL	-	expression tag	UNP P42212
A	243	LEU	-	expression tag	UNP P42212
A	244	PHE	-	expression tag	UNP P42212
A	245	GLN	-	expression tag	UNP P42212
A	246	GLY	-	expression tag	UNP P42212
A	247	PRO	-	expression tag	UNP P42212
A	248	SER	-	expression tag	UNP P42212
A	249	HIS	-	expression tag	UNP P42212
A	250	HIS	-	expression tag	UNP P42212
A	251	HIS	-	expression tag	UNP P42212
A	252	HIS	-	expression tag	UNP P42212
A	253	HIS	-	expression tag	UNP P42212
A	254	HIS	-	expression tag	UNP P42212

- Molecule 2 is a protein called LaG41.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	125	Total	C	H	N	O	S	0	0	0
			1883	596	926	169	187	5			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		

i

- Molecule 1: Green fluorescent protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	108.63Å 108.63Å 198.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 3.11 47.19 – 3.11	Depositor EDS
% Data completeness (in resolution range)	83.6 (47.19-3.11) 83.6 (47.19-3.11)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158)	Depositor
R, R_{free}	0.273 , 0.303 0.272 , 0.302	Depositor DCC
R_{free} test set	1987 reflections (8.40%)	wwPDB-VP
Wilson B-factor (Å ²)	73.0	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.100 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5445	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CR2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/1839	0.43	0/2485
2	B	0.16	0/974	0.44	0/1317
All	All	0.17	0/2813	0.43	0/3802

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	124	GLY	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1816	1740	1757	48	2
2	B	957	926	926	31	2
3	A	6	0	0	0	0
All	All	2779	2666	2683	76	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 76 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:ILE:HD11	2:B:73:ARG:HB2	1.64	0.79
1:A:113:LYS:HE3	1:A:188:ILE:HD13	1.65	0.78
2:B:32:THR:HG21	2:B:99:ALA:HB1	1.67	0.76
1:A:96:ARG:HB2	1:A:183:GLN:HB3	1.66	0.75
1:A:163:VAL:HG23	1:A:183:GLN:HG3	1.68	0.74

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLU:OE1	2:B:107:THR:OG1[7_454]	2.08	0.12
1:A:45:LYS:NZ	2:B:111:ASP:OD2[7_454]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/253 (88%)	218 (98%)	4 (2%)	0	100	100
2	B	123/141 (87%)	118 (96%)	3 (2%)	2 (2%)	7	29
All	All	345/394 (88%)	336 (97%)	7 (2%)	2 (1%)	21	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	125	LEU
2	B	124	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/219 (90%)	196 (100%)	1 (0%)	81	83
2	B	100/114 (88%)	100 (100%)	0	100	100
All	All	297/333 (89%)	296 (100%)	1 (0%)	86	86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	A	157	GLN
2	B	40	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CR2	A	66	1	20,20,21	2.84	8 (40%)	25,27,29	2.57	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR2	A	66	1	-	1/6/25/26	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CR2	C1-N2	6.10	1.42	1.32
1	A	66	CR2	CA2-C2	5.54	1.54	1.48
1	A	66	CR2	C1-N3	5.53	1.46	1.37
1	A	66	CR2	C2-N3	3.82	1.48	1.40
1	A	66	CR2	CG2-CB2	3.69	1.53	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	CR2	O2-C2-CA2	-8.16	125.81	131.02
1	A	66	CR2	C2-N3-C1	-6.55	105.13	108.08
1	A	66	CR2	CA2-C2-N3	4.38	107.18	103.50
1	A	66	CR2	CG2-CB2-CA2	-3.10	126.18	129.87
1	A	66	CR2	C2-CA2-N2	-3.01	106.79	108.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CR2	C3-CA3-N3-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CR2	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	226/253 (89%)	0.44	8 (3%)	47	27	53, 79, 110, 132	0
2	B	125/141 (88%)	0.53	6 (4%)	35	19	64, 89, 128, 150	0
All	All	351/394 (89%)	0.48	14 (3%)	42	23	53, 83, 120, 150	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	125	LEU	4.7
1	A	205	SER	3.7
1	A	145	TYR	3.5
2	B	127	VAL	3.3
1	A	149	ASN	3.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CR2	A	66	19/20	0.88	0.20	41,67,86,89	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.